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Phase determination for the strychnine sulfonic acid tetrahydrate by direct methods using the role of structure invariants*

S. NATARAJAN** AND DODDAHALLI S. SAKEGOWDA***

Material Science Division, Department of Mechanical Engineering, 1515 West Wisconsin Avenue, Milwaukee, Wisconsin 53233, *U.S.A.*

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Phases were specified to fix the origin and enantiomorph and some derived using $\Sigma 1$ relations and pair relations. Using the basic set of phases and the cosine values of the associated structure invariants, an initial set of 52 phases were obtained. This was used as input in the tangent formula so that a total of 295 phases were derived. On computing an E-map, 28 nonhydrogen atoms out of 33 were obtained.

1. INTRODUCTION

Since 1969 a number of structures have been solved by direct methods using the cosine values of the structure invariants, $\cos(\phi_{\boldsymbol{h}_1}+\phi_{\boldsymbol{h}_2}+\phi_{\boldsymbol{h}_3})$, where $\boldsymbol{h}_1+\boldsymbol{h}_2+\boldsymbol{h}_3=0$, first described by Karle & Hauptman (1957). The structure of strychnine sulfonic acid tetrahydrate $C_{21}H_{22}N_2O_2 \cdot SO_3, 4H_2O$ has also been solved by the above method. Strychnine sulfonic acid tetrahydrate crystallizes in space group $P2_12_12_1$ with one molecule in the asymmetric unit. The cell dimensions are

$$a = 14{\cdot}007 \pm 0{\cdot}004\text{Å},$$
$$b = 20{\cdot}379 \pm 0{\cdot}005\text{Å},$$
$$c = 7{\cdot}441 \pm 0{\cdot}003\text{Å}.$$

The present paper describes the procedure used to obtain an initial set of about 52 phases for solving the structure. The initial set of phases consists of those specified to fix the origin and enantiomorph (Hauptman *et al* 1956) and those derived using the $\Sigma 1$ relations (Hauptman *et al* 1953) and also pair relations

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Present address of the authors :

** C.S.I.R. Pool Officer, Department of Physics, Madurai University, Madurai, Madras-625021.

*** Department of Physics, Central College, Bangalore University, Bangalore.

(Hauptman 1972) which together form the basic set of phases. Corresponding to each distinct pair ϕ_k, ϕ_{-h-k} (where $\phi_k = \phi_{h_2}$, $\phi_{-h-k} = \phi_{h_3}$) of the basic set, the permissible phase ϕ_h $(= \phi_{h_1})$ is found using the cosine value of the associated structure invariant $\phi_h+\phi_k+\phi_{-h-k}$. The new phase ϕ_h is added to the basic set of known phases and the process repeated to obtain an initial set of about 52 phases. The initial set of phases thus obtained are used as input in the tangent formula (Hauptman *et al* 1956) which is used to determine about 243 additional phases. Subsequently, 28 of the nonhydrogen atoms were found from the E-map based on all 295 phases. The details of the structure has been published by Sakegowda, Cartz & Natarajan (1973).

2. Structure Analysis

The two dimensional reflections with their normalized structure factors $|E|_{obs} > 1{\cdot}5$ are given in table 1. The values of three linearly independent phases of reflections from this table are arbitrarily specified thus fixing the origin. One more phase is arbitrarily specified to fix the enantiomorph. The origin vectors and enantiomorph vector are so chosen that their normalized structure factors are large and will interact with many triplets having large $|E_1E_2E_3|$ values. Table 2 shows the assignment of origin and enantiomorph.

In space $P2_12_12_1$, $\Sigma 1$ relations are used to find the phases of the type $\phi(2h, 2k, 0)$, $\phi(2h, 0, 2l)$ and $\phi(0, 2k, 2l)$. The $\Sigma 1$ indications for reflections having $|E|_{obs} > 1{\cdot}5$ are shown in table 3. A phase is considered to be determined if its probability value is greater than 75% and having large E_{calc} value. Using this criterion, the phases of the reflections (12, 0, 0), (6, 20, 0) and (4, 8, 0) are added to the basic set, and $\pi, 0, \pi$ are the phase of (12, 0, 0), (6, 20, 0) and (4, 8, 0) reflections derived from $\Sigma 1$ relations. Table 3 also gives the true phases of the reflections derived from the structure.

In addition, pair relations have proved useful in deriving the phases of several important reflections. In space group $P2_12_12_1$ the two types of paired formulae that exist allow the cosine seminvariants $\cos(\phi_1+\phi_2)$ to be computed from the normalized structure factors. In table 4, the data for 56 pairs are presented out of 207 between strongest two dimensional reflections needed in phase determination. They are listed in the order in which the phases are derived. A few pairs play a secondary role in that they provided supporting evidence with two dimensional and three dimensional triplets.

In determining phases using pairs, a few conflicts are observed. For example, (0, 19, 1) pair with (0, 13, 3). There is a strong indication that $\phi(0, 19, 1)$ should be $\pi/2$. However, (0, 1, 5) pairs with (0, 13, 3) and (0, 7, 3), and $\phi(0, 1, 5)$ should be $\pi/2$, so that there is a reasonable indication to believe that $\phi(0, 19, 1)$ should be $-\pi/2$. Again (0, 17, 1) pairs with (0, 7, 3) and (0, 19, 1), and (0, 17, 5) pairs with (0, 17, 1) and (0, 19, 1). The conflicts are lessened by accepting the phase of $\phi(0, 19, 1)$ as $\pi/2$.

Table 1. Two dimensional reflections with $|E|_{obs} > 1{\cdot}5$ arranged according to parity

0	g	g	|E|	0	g	u	|E|	0	u	g	|E|
				0	20	1	2.921	0	7	2	2.148
0	16	2	2.431	0	16	1	2.430	0	1	4	2.007
0	12	6	2.032	0	18	3	2.156	0	9	4	1.684
0	6	2	1.967	0	8	7	1.683	0	3	6	1.608
0	6	4	1.905	0	4	5	1.678				
0	16	4	1.858	0	14	3	1.543				
0	8	2	1.628	0	6	5	1.506				
0	6	6	1.503								

0	u	u	|E|	g	0	g	|E|	g	0	u	|E|
0	13	3	2.448	2	0	2	1.529	10	0	3	1.984
0	17	5	2.211	12	0	2	1.500	14	0	5	1.924
0	19	1	1.993					6	0	5	1.615
0	1	5	1.877								
0	5	7	1.861								
0	17	1	1.838								
0	7	3	1.786								

u	0	g	|E|	u	0	u	|E|	g	g	0	|E|
13	0	6	2.373	3	0	5	1.576	2	16	0	2.700
13	0	4	1.904					14	10	0	2.626
11	0	4	1.809					4	8	0	2.155
7	0	4	1.635					6	12	0	2.073
								12	0	0	2.072
								12	8	0	1.792
								12	4	0	1.684

g	u	0	|E|	u	g	0	|E|	u	u	0	|E|
6	17	0	2.224	1	18	0	2.704	9	11	0	2.475
8	15	0	2.184	5	6	0	2.269	7	5	0	2.308
12	13	0	2.043	9	12	0	2.019	9	19	0	1.989
14	11	0	2.017	5	10	0	2.012	3	9	0	1.979
6	7	0	1.977	3	20	0	1.808	9	7	0	1.927
12	3	0	1.831	7	2	0	1.690	11	17	0	1.699
10	15	0	1.750	3	6	0	1.624	11	3	0	1.615
8	11	0	1.638	11	16	0	1.589				
4	5	0	1.621	13	6	0	1.546				
12	17	0	1.598								
6	5	0	1.578								

Table 2. Assignment of origin and enantiomorph

h			$\|E\|$	ϕ	
0	13	3	2.448	$\pi/2$	origin specification
0	16	1	2.430	0	
7	5	0	2.308	$-\pi/2$	
1	18	0	2.704	$\pi/2$	enantiomorph

Table 3. $\Sigma 1$ results for strychnine sulfonic acid tetrahydrate

h			$\|E\|_{obs}$	E_{calc}	$P_+(E_{\boldsymbol{h}})$	True phase
12	0	0	2.07	−4.07	0.06	π
12	4	0	1.68	1.62	0.57	0
4	8	0	2.16	−4.84	0.23	π
12	8	0	1.79	1.14	0.55	0
14	10	0	2.63	−2.21	0.35	π
2	16	0	2.70	−2.24	0.35	π
6	20	0	2.07	8.16	0.85	0
2	0	2	1.53	−2.03	0.32	π
12	0	2	1.50	−0.47	0.46	π
0	6	2	1.97	1.91	0.66	0
0	8	2	1.63	−0.55	0.46	π
0	16	2	2.43	−1.54	0.34	0
0	6	4	1.91	1.86	0.65	0
0	16	4	1.86	3.01	0.73	0
0	6	6	1.50	−2.73	0.33	π
0	12	6	2.03	1.10	0.60	π

Table 4. $\Sigma 2$ triplets for large contributors (both $A > 1$) for selected pairs.

Sl. No.	$\boldsymbol{h}_1$			$\boldsymbol{h}_2$			$\boldsymbol{h}_3$			$\boldsymbol{h}_4$			$A(134)$	$A(234)$	*CTR*
42	0	16	1	0	8	7	5	12	4	5	4	3	1.54	1.07	−135.0
43	0	16	1	0	8	7	11	12	4	11	4	3	1.93	1.33	−314.0
51	0	20	1	0	8	7	0	14	3	0	6	4	1.84	1.06	−157.0
52	0	20	1	0	8	7	8	14	3	8	6	4	2.23	1.28	−269.0
53	0	20	1	0	8	7	10	14	3	10	6	4	2.02	1.16	−212.0
35	0	16	1	0	18	3	0	17	1	0	1	2	1.27	1.12	77.0
36	0	16	1	0	18	3	12	17	1	12	1	2	2.22	1.97	455.0
44	0	20	1	0	18	3	0	19	1	0	1	2	1.65	1.22	96.0
37	0	16	1	0	4	5	6	10	3	6	6	2	1.45	1.00	137.0
38	0	16	1	0	4	5	10	10	3	10	6	2	1.50	1.04	148.0
39	0	16	1	0	4	5	12	10	3	12	6	2	1.62	1.12	186.0
45	0	20	1	0	4	5	9	12	2	9	8	3	2.69	1.54	466.0
46	0	20	1	0	4	5	11	12	2	11	8	3	2.19	1.26	242.0

Table 4. (*contd.*) $\Sigma 2$ triplets for large contributors (both $A > 1$) for selected pairs

Sl. No.	h_1			h_2			h_3			h_4			$A(134)$	$A(234)$	CTR
87	0	7	3	0	13	3	12	10	3	12	3	0	1.39	1.91	−300.0
88	0	7	3	0	13	3	2	10	0	2	3	3	1.10	1.51	−139.0
89	0	7	3	0	13	3	14	10	0	14	3	3	1.26	1.76	−149.0
90	0	7	3	0	1	5	12	4	4	12	3	1	1.52	1.59	−365.0
95	0	13	3	0	1	5	10	7	1	10	6	4	1.39	1.06	116.0
96	0	13	3	0	1	5	12	7	1	12	6	4	2.42	1.85	550.0
80	0	19	1	0	13	3	11	16	2	11	3	1	1.27	1.56	165.0
81	0	19	1	0	13	3	13	16	1	13	3	2	1.23	1.51	147.0
82	0	19	1	0	1	5	8	10	3	8	9	2	1.08	1.02	−100.0
83	0	19	1	0	1	5	10	10	3	10	9	2	1.14	1.08	−112.0
84	0	19	1	0	1	5	10	14	3	14	9	2	1.12	1.06	−104.0
47	0	20	1	0	6	5	0	13	3	0	7	2	3.30	1.70	−780.0
48	0	20	1	0	6	5	12	13	3	12	7	2	2.20	1.13	−273.0
49	0	20	1	0	6	5	3	13	2	3	7	3	2.16	1.11	−246.0
56	0	18	3	0	6	5	8	12	1	8	6	4	2.45	1.71	−796.0
198	7	5	0	9	11	0	8	8	2	1	3	2	1.21	1.29	−88.0
199	7	5	0	9	11	0	8	8	4	1	3	4	1.26	1.36	−99.0
200	7	5	0	9	11	0	8	3	6	1	8	6	1.00	1.08	−45.0
74	0	17	1	0	7	3	8	12	1	8	5	2	1.16	1.13	−105.0
72	0	17	1	0	19	1	0	18	3	0	1	2	1.12	1.22	118.0
73	0	17	1	0	19	1	0	18	3	0	1	4	1.71	1.85	478.0
85	0	19	1	0	17	5	0	18	3	0	1	2	1.22	1.35	−118.0
76	0	17	1	0	17	5	1	17	3	1	0	2	1.06	1.28	−112.0
77	0	17	1	0	17	5	0	18	3	0	1	2	1.12	1.35	−118.0
78	0	17	1	0	17	5	0	13	3	0	4	2	1.44	1.73	264.0
50	0	20	1	0	20	5	0	13	3	0	7	2	3.30	1.65	−780.0
60	0	6	5	0	20	5	0	13	3	0	7	2	1.70	1.65	780.0
57	0	18	3	0	20	5	0	19	1	0	1	4	1.85	1.25	380.0
10	0	6	2	0	16	2	7	11	2	7	5	0	1.62	2.01	334.0
11	0	6	2	0	16	2	13	11	2	13	5	0	1.00	1.23	66.0
12	0	16	2	0	16	2	9	11	0	9	5	2	1.95	2.41	542.0
4	0	4	2	0	6	2	12	5	0	12	1	2	1.02	1.35	−180.0
5	0	4	2	0	6	2	0	5	7	0	1	5	1.12	1.47	−268.0
68	0	9	4	0	3	6	9	6	5	9	3	1	1.39	1.33	348.0
69	0	9	4	0	3	6	11	6	5	11	3	1	1.19	1.13	226.0
180	7	2	0	1	18	0	4	8	1	3	10	1	1.33	2.13	−296.0
193	11	3	0	7	3	0	9	19	0	2	16	0	1.86	1.63	803.0
194	11	3	0	9	11	0	10	7	3	1	4	3	1.10	1.68	201.0
189	5	10	0	1	18	0	3	14	5	2	4	5	1.13	1.52	−111.0
182	3	6	0	3	20	0	3	13	2	0	7	2	1.20	1.34	247.0
183	3	6	0	3	20	0	3	7	3	0	13	3	1.83	2.04	778.0
184	3	6	0	3	20	0	12	13	0	9	7	0	1.37	1.52	372.0
190	5	10	0	3	20	0	4	5	4	1	15	4	1.14	1.02	92.0

There are three indications to show that $\phi(0,17,5)$ should be $-\pi/2$ and one indication that it should be $+\pi/2$. Similarly, there is a strong indication that $\phi(0,20,5)$ should be π and one weak indication to show that it should be zero. The conflicts are resolved by changing the sign of the cosines wherever necessary. This is strongly favoured since the triple product and the *MDKS* values for $\cos[\phi(0,17,1)+\phi(0,\mathbf{4},2)+\phi(0,\mathbf{13},\mathbf{3})]$ and $\cos[\phi(0,20,5)+\phi(0,\mathbf{19},\mathbf{1})+\phi(0,\mathbf{1},\mathbf{4})]$ are lower. Table 5 shows that the sets of cosines forming contributions to the respective pairs indicate that certain cosines be negative.

Table 5. Low *TPROD* and *MDKS* values in conflicting $\Sigma 2$ triplets

$h(h_1$ or $h_2)$	$k(h_3)$	$-h-k(h_4)$	A	$\cos(\phi_h+\phi_k+\phi_{-h-k})$ *TPROD*	$\cos(\phi_h+\phi_k+\phi_{-h-k})$ *MDKS*	*CTR*
0 17 1	0 4 2	0 13 3	1.44	−0.95	−0.06	264.0
0 17 5	0 4 2	0 13 3	1.73	0.75	0.83	264.0
0 18 3	0 19 1	0 1 4	1.85	1.13	−0.31	389.0
0 20 5	0 19 1	0 1 4	1.25	0.07	0.30	389.0

Sixteen $\Sigma 2$ triplets which involve two dimensional reflections out of 186 needed in phase determination are presented in Table 6 and 23 of those out of 528 which involve three dimensional reflections are presented in Table 7. The cosine

Table 6. Cosine triplets for two dimensional reflections with $A > 1$ needed for phase determination

Sl. No.	h	k	$-h-k$	Signs	*TPS*	A	*TPROD*	*MDKS*
2	0 20 1	0 7 2	0 13 3	+ + −	0	3.30	2.12	2.22
40	0 7 2	0 13 3	0 6 5	+ + −	0	1.70	2.51	1.31
46	0 7 2	0 13 3	0 20 5	+ + −	0	1.65	1.80	0.82
11	0 20 1	0 12 6	0 8 7	+ + −	0	2.14	1.38	1.20
34	0 16 1	0 4 5	0 12 6	+ + −	0	1.78	1.11	0.77
1	7 5 0	9 11 0	2 16 0	+ − +	0	3.31	1.02	1.39
23	0 7 2	0 16 2	0 9 4	+ + −	0	1.89	1.52	1.03
7	0 20 1	0 17 5	0 3 6	+ + −	π	2.23	2.46	2.27
144	0 6 2	0 9 4	0 3 6	+ + −	0	1.14	0.92	0.86
14	7 2 0	1 18 0	6 20 0	+ − −	π	2.03	1.43	1.29
10	2 16 0	2 0 2	0 16 2	+ − +	0	2.15	1.85	1.39
21	0 20 1	0 6 2	0 14 3	+ + −	0	1.90	1.21	1.60
68	0 8 0	9 11 0	9 19 0	+ + −	0	1.45	1.14	1.34
49	7 3 0	2 16 0	9 19 0	+ + −	0	1.63	2.06	1.29
4	4 8 0	5 10 0	1 18 0	+ − +	0	2.52	0.61	0.64
22	3 6 0	5 10 0	2 16 0	+ − +	π	1.89	1.82	0.78

Table 7. Cosine triplets for three dimensional reflections with $A > 1$ needed for phase determination

Sl. No.	h			k			$-h-k$			Signs	TPS	A	$\cos(\phi_h+\phi_k+\phi_{-h-k})$ TPROD	MDKS
19	2	16	0	2	3	3	0	13	3	+ − +	π	2.80	1.06	1.19
139	1	18	0	1	6	6	0	12	6	+ − +	0	2.20	1.46	1.44
27	9	11	0	9	8	1	0	19	1	+ − −	π	2.71	1.15	1.24
52	9	8	1	9	5	2	0	13	3	+ − −	0	2.50	1.27	1.48
309	9	11	0	9	5	2	0	6	2	+ − +	0	1.94	0.80	0.97
14	9	8	1	0	16	2	9	8	3	+ + +	π	2.92	1.00	0.59
173	7	5	0	2	3	3	9	8	3	+ + −	0	2.14	1.45	1.07
96	7	5	0	9	8	3	2	13	3	+ − +	0	2.31	1.42	1.22
13	2	16	0	9	8	3	11	8	3	+ + +	π	2.94	1.28	1.39
70	9	11	0	2	3	3	11	8	3	+ + +	π	2.43	0.84	0.79
49	1	18	0	11	8	3	10	10	3	+ − −	π	2.54	1.73	0.99
76	1	18	0	9	8	3	10	10	3	+ + +	0	2.40	1.02	0.99
311	9	8	1	2	0	2	11	8	3	+ + −	0	1.94	2.52	1.72
87	11	8	3	0	13	3	11	5	6	+ + +	0	2.35	1.01	1.13
277	1	18	0	9	8	3	8	10	3	+ − −	π	1.96	1.19	0.72
8	9	8	1	0	20	1	9	12	2	+ + +	π	3.14	1.50	0.98
31	0	20	1	9	12	2	9	8	3	+ + +	0	2.09	0.59	0.88
40	5	10	0	5	10	1	0	20	1	+ − −	π	2.59	0.81	0.98
476	12	0	0	0	7	2	12	7	2	+ + −	0	1.83	2.11	1.62
475	5	10	0	2	3	3	3	7	3	+ − +	0	1.83	1.69	1.49
470	3	6	0	3	7	3	0	13	3	+ − −	0	1.83	1.18	1.51
92	8	15	0	3	7	3	11	8	3	+ + +	0	2.33	1.25	1.00
16	8	15	0	8	5	1	0	20	1	+ − −	π	2.87	1.71	1.58

invariants corresponding to each of these triplets are computed by means of the triple product (Hauptman 1964) and the *MDKS* formulae (Hauptman 1972) using thresholds of 2·0 and 1·3, respectively. The triple product scaling parameter has a value of 1350·0 and scaling parameters M and K used in the *MDKS* formula have values of 6·55 and 0·40, respectively. The set of initial phases assigned and the reason for their assignment are given in Table 8.

3. Conclusion

In solving the structure of strychnine sulfonic acid tetrahydrate, pair relations have proved to be useful in obtaining the initial phases of about a dozen important reflections. Cosine invariants for triplets involving three dimensional reflections are also used in the phase determination and the phases of about 15 three dimensional reflections are derived before using the tangent formula for phase extension and refinement.

Table 8. Initial phases for strychnine sulfonic acid tetrahydrate in the order in which they were determined

Sl. No.	h			$\|E\|$	Derived Phase $\times\pi$	Reason	True Phase $\times\pi$
1	0	13	3	2.448	0.50		0.50
2	0	16	1	2.430	0.00	Origin	0.00
3	7	5	0	2.308	−0.50		−0.50
4	1	18	0	2.704	0.50	Enantiomorph	0.50
5	12	0	0	2.072	1.00		1.00
6	4	8	0	2.155	1.00	Σ Relationship	1.00
7	6	20	0	2.073	0.00		0.00
8	0	8	7	1.683	1.00	Pair with (0, 16, 1)	1.00
9	0	20	1	2.921	0.00	Pair with (0, 8, 7)	0.00
10	0	18	3	2.156	0.00	Pairs with (0, 16, 1) and (0, 20, 1)	0.00
11	0	4	5	1.678	0.00	Pairs with (0, 16, 1) and (0, 20, 1)	0.00
12	0	7	3	1.786	−0.50	Pair with (0, 13, 3)	−0.50
13	0	1	5	1.877	0.50	Pairs with (0, 13, 3) and (0, 7, 3)	0.50
14	0	19	1	1.993	0.50	Pairs with (0, 13, 3) and (0, 1, 5)	0.50
15	0	6	5	1.506	1.00	Pairs with (0, 18, 3) and (0, 20, 1)	1.00
16	9	11	0	2.475	0.50	Pair with (7, 5, 0)	0.50
17	0	17	1	1.838	0.50	Pairs with (0, 7, 3) and (0, 19, 1)	0.50
18	0	17	5	2.211	−0.50	Pairs with (0, 19, 1) and (0, 17, 1)	−0.50
19	0	7	2	2.148	0.50	2D Triples 2 and 40	0.50
20	0	20	5	1.460	1.00	Pairs with (0, 20, 1), (0, 6, 5) and (0, 18, 3); 2D Triple 46	1.00
21	0	12	6	2.032	1.00	2D Triples 11, 34	1.00
22	2	16	0	2.700	1.00	2D Triple 1	1.00
23	2	3	3	1.973	−0.50	3D Triple 19	0.70
24	1	6	6	1.869	0.50	3D Triple 139	−0.58
25	9	8	1	2.558	1.00	3D Triple 27	0.99
26	9	5	2	1.862	0.50	3D Triple 52	0.45
27	0	6	2	1.967	0.00	3D Triple 309; Σ1	0.00
28	0	16	2	2.431	0.00	Pair with (0, 6, 2)	0.00
29	0	4	2	1.490	1.00	Pair with (0, 6, 2)	1.00
30	9	8	3	2.190	0.00	3D Triples 14, 173	−0.04
31	2	13	3	2.131	0.50	3D Triple 96	0.44
32	0	9	4	1.684	0.50	2D Triple 23	0.50
33	0	3	6	1.608	0.50	Pair with (0, 9, 4); 2D Triples 7 and 144	0.50
34	7	2	0	1.690	−0.50	Pair with (1, 18, 0); 2D Triple 14	−0.50
35	11	8	3	2.315	0.00	3D Triples 13 and 70	−0.15

Table 8 (Contd.)

Sl. No.	h			E	Derived Phase × π	Reasons	True Phase × π
36	10	10	3	1.892	−0.50	3D Triples 49 and 76	−0.24
37	2	0	2	1.529	1.00	2D Triple 10; 3D Triple 311	1.00
38	11	5	6	1.930	−0.50	3D Triple 87	−0.48
39	8	10	3	1.542	−0.50	3D Triple 277	−0.53
40	0	14	3	1.543	0.00	2D Triple 21	0.00
41	9	12	2	1.960	0.00	3D Triples 8 and 31	−0.50
42	9	19	0	1.989	−0.50	2D Triple 68	−0.50
43	7	3	0	1.482	0.50	2D Triple 49	0.50
44	11	3	0	1.615	0.50	Pairs with (7, 3, 0) and (9, 11, 0)	0.50
45	5	10	0	2.012	−0.50	Pair with (1, 18, 0); 2D Triple 4	−0.50
46	5	10	1	2.052	0.50	3D Triple 40	0.51
47	12	7	2	1.920	−0.50	3D Triple 476	−0.49
48	3	7	3	2.144	1.00	3D Triple 475	1.08
49	3	6	0	1.624	−0.50	3D Triple 470 and 2D Triple 22	−0.50
50	3	20	0	1.808	−0.50	Pairs with (3, 6, 0) and (5, 10, 0)	−0.50
51	8	15	0	2.184	1.00	3D Triple 92	1.00
52	8	5	1	2.092	0.00	3D Triple 16	0.075

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